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COUPLED NEUTRONICS AND THERMAL-HYDRAULIC SOLUTION OF A FULL-CORE PWR USING VERA-CS

Scott Palmtag
Core Physics, Inc.
Wilmington, North Carolina, USA
scott.palmtag@corephysics.com

Kevin Clarno, Greg Davidson, Robert Salko, Tom Evans, John Turner
Oak Ridge National Laboratory
Oak Ridge, Tennessee, USA
clarnokt@ornl.gov
davidsongg@ornl.gov
salkork@ornl.gov
evanstm@ornl.gov
turnerja@ornl.gov

Kenneth Belcourt, Russell Hooper, Rod Schmidt
Sandia National Laboratories
Albuquerque, New Mexico, USA
kbelco@sandia.gov
rhoope@sandia.gov
rcschmi@sandia.gov

ABSTRACT

The Consortium for Advanced Simulation of Light Water Reactors (CASL) is developing a core simulator called VERA-CS to model operating PWR reactors with high resolution. This paper describes how the development of VERA-CS is being driven by a set of progression benchmark problems that specify the delivery of useful capability in discrete steps. As part of this development, this paper will describe the current capability of VERA-CS to perform a multiphysics simulation of an operating PWR at Hot Full Power (HFP) conditions using a set of existing computer codes coupled together in a novel method. Results for several single-assembly cases are shown that demonstrate coupling for different boron concentrations and power levels. Finally, high-resolution results are shown for a full-core PWR reactor modeled in quarter-symmetry.

Key Words: **Core Simulator, Multiphysics, Neutron Transport, Subchannel Thermal-Hydraulics.**

1. INTRODUCTION

The Consortium for Advanced Simulation of Light Water Reactors (CASL) is the first DOE Energy Innovation Hub. CASL was established in July 2010 for the purpose of providing advanced modeling and simulation (M&S) solutions for commercial nuclear reactors [1]. CASL's vision is to predict, with confidence, the performance of nuclear reactors through comprehensive, science-based modeling and simulation technology that is deployed and applied broadly throughout the nuclear energy industry to enhance safety, reliability, and economics.

An important part of CASL is the Virtual Environment for Reactor Applications (VERA), which is a M&S environment which provides higher-fidelity results than the current industry approaches by incorporating coupled physics and science-based models, state-of-the-art numerical methods, and modern computational science and world-class computing facilities.

One part of the VERA environment is the VERA Core Simulator (VERA-CS). VERA-CS is a base technology needed to model operating reactors throughout their lifetime to provide high-fidelity results to support the solution of Challenge Problems such as CRUD Induced Power Shift (CIPS), CRUD Induced Local Corrosion (CILC), Pellet Clad Interaction (PCI), and Grid to Rod Fretting (GTRF).

VERA-CS is currently under development and this paper describes the development process and demonstrates the multiphysics coupling capability used to model full-core reactors at Hot Full Power (HFP) conditions. The multiphysics coupling includes the coupling of several existing computer codes. Cross sections are obtained from XSProc, which is a component of the SCALE cross section package from ORNL. Neutron transport is provided by the Insilico code from ORNL, and the thermal-hydraulic solution is provided by the COBRA-TF (CTF) code being developed at Penn State University (PSU). The coupling and management of these codes as a single application is done with the LIME toolkit, and the Data Transfer Toolkit (DTK) is used to transfer solution data between the different codes.

Future development of VERA-CS will include the addition of depletion capabilities using the ORIGEN code from ORNL, detailed chemistry models using MAMBA from LANL, and detailed fuel performance models using the Moose/Bison code from INL.

1.1 Progression Benchmark Problems

To guide the development of VERA-CS, a set of ten CASL Progression Benchmark Problems have been developed to define requirements and prioritize capabilities [2]. The progression problems define useful capability in discrete steps ranging from a single pincell up to full-core depletion. The progression problems guide priorities and provide specific deliveries when users can start verification and validation studies of completed components.

The CASL Progression Benchmark Problems are listed in Table 1-1. Reference [3] (presented at this conference) describes the completion and validation of Progression Problem 5. This paper describes the completion of Problems 6 and 7.

Table 1-1 CASL Progression Benchmark Problems

•#1 2D HZP Pincell
•#2 2D HZP Lattice
•#3 3D HZP Assembly
•#4 HZP 3x3 Assembly CRD Worth
•#5 Physical Reactor Zero Power Physics Tests (ZPPT)
•#6 HFP BOL Assembly (with boron search)
•#7 HFP BOC Physical Reactor
•#8 Physical Reactor Startup Flux Maps
•#9 Physical Reactor Depletion
•#10 Physical Reactor Refueling

Progression problems 1-5 are at hot zero power (HZP) conditions and do not include thermal-hydraulic feedback. Problems 6 and 7 are the first progression problems that couple neutronic and thermal-hydraulic solutions.

2. PHYSICS COMPONENT DESCRIPTIONS

This section includes descriptions of the individual physics components (CTF and Insilico) and the VERA Common Input module.

2.1 VERA Common Input (VERAIn)

The VERA Common Input (VERAIn) is a single common input used to drive all of the physics codes in the VERA Core Simulator (VERA-CS). Early in the development of the core simulator, it was recognized that it would be unreasonable to require users to generate input decks for each of the individual physics codes. This is especially true if the core simulator allows multiple codes to solve each physics problem (i.e. multiple subchannel codes, multiple neutronics solvers). In addition to the ease-of-use aspects, it is critical in multiphysics applications that all of the different code systems have consistent input. Having a single common input simplifies the user experience and helps ensure that all of the physics applications are solving a consistent geometry.

The common input is based on a single ASCII input file. The input file uses a free-form input format that is based on keyword inputs. The format of the input file was designed by engineers with broad experience with current industry core design tools, so the format of the input file will be easy for industry users to understand. The ASCII input file provides several advantages to the users:

- Allows users to easily transfer input and output between different computer systems.
- Allows users ability to easily edit the file on remote computers.
- Provides a format that users can readily read and understand.
- Provides an approved archive format recognized by the NRC.
- Allows users to “diff” input files on a variety of remote computers.
- Allows users to archive inputs in standard source code repositories and/or directories with read-only permissions.

The input file contains a description of the physical reactor geometry, including: fuel assemblies, removable poison assemblies, control rods, non-fuel structures, detectors, baffle, etc. The input file also contains a description of the current reactor statepoint including power, flow, depletion, search options, etc.

In order to translate the user input to input needed for the individual code packages, a multistep process is used. First, an input parser reads the text input file and converts it into an XML file. Some physics codes, such as Insilico and MPACT, can read the XML file directly using readily-available XML libraries. Other codes, such as CTF and Peregrine, require an intermediate step that converts the XML file into the native code input. This process allows the common input file to be used for existing physics codes where we do not want to make extensive modifications to the input.

Currently, the following physics codes can interface with the VERA common input:

- Insilico
- MPACT
- COBRA-TF (CTF)
- Peregrine

Examples of VERA common input files are shown in References [4] and [5].

It should be noted that there is one class of input that cannot be readily generated by the VERA common input. Some physics codes, such as CFD, require a detailed mesh that is usually generated from a CAD file. For these codes, it is expected that the user will still have to attach an externally generated mesh file and make sure that the mesh file is consistent with the common input.

2.2 COBRA-TF (CTF)

COBRA-TF (CTF) is a thermal-hydraulic simulation code designed for Light Water Reactor (LWR) analysis) [6]. CTF has a long lineage that goes back to the original COBRA program developed in 1980 by Pacific Northwest Laboratory under sponsorship of the Nuclear Regulatory Commission (NRC). The original COBRA began as a thermal-hydraulic rod-bundle analysis code, but versions of the code have been continually updated and expanded over the past several decades to cover almost all of the steady-state and transient analysis of both PWR's and BWR's. CTF is currently being developed and maintained by the Reactor Dynamics and Fuel Management Group (RDFMG) at the Pennsylvania State University (PSU).

CTF includes a wide range of thermal-hydraulic models important to LWR safety analysis including flow regime dependent two-phase wall heat transfer, inter-phase heat transfer and drag, droplet breakup, and quench-front tracking. CTF also includes several internal models to help facilitate the simulation of actual fuel assemblies. These models include spacer grid models, a fuel rod conduction model, and built-in material properties for both the structural materials and the coolant (i.e. steam tables).

CTF uses a two-fluid, three-field representation of the two-phase flow. The equations and fields solved are:

- Continuous vapor (mass, momentum and energy)
- Continuous liquid (mass, momentum and energy)
- Entrained liquid drops (mass and momentum)
- Non-condensable gas mixture (mass)

Some of the reasons for selecting CTF as the primary T/H solver in the VERA core simulator are the reasonable run-times compared to CFD (although CFD will be available as an option), the fact that it is being actively developed and supported by PSU, and for the ability to support future applications of VERA such as transient safety analysis and BWR and SMR applications.

Since incorporating CTF into VERA, additional work has been done to allow CTF to run full-core problems on parallel computers using a domain decomposition model [7].

2.3 Insilico

Insilico is one of the neutronics solvers in the VERA Core Simulator (along with MPACT) and is part of the Exnihilo transport suite being developed by ORNL. Insilico is the reactor toolkit package of Exnihilo and includes the reactor toolkit used for meshing of PWR geometry, and the cross section generation package based on XSProc. Insilico uses the Denovo module [8][9] to solve for the flux and eigenvalue solutions of the 3D problem using either the discrete ordinates (S_N) solver or the Simplified Legendre (SP_N) solver. Exnihilo also includes the SHIFT Monte Carlo package, but SHIFT is not used in this study.

Multigroup cross sections are generated in Insilico using the SCALE [10] code XSProc. XSProc performs resonance self-shielding with full range Bondarenko factors using either the narrow resonance approximation or the intermediate resonance approximation. The fine energy group structure of the resonance self-shielding calculation can optionally be collapsed to a coarse group structure through a one-dimensional (1D) discrete ordinates transport calculation internal to XSProc. The cross section collapse is general, but for all of the calculations in this study, the fine energy group structure is collapsed to a 11-group or 23-group coarse group structure to be used in the Denovo 3D transport solver.

The cross section libraries used in this study are the SCALE 6.2 252-group and 56-group ENDF/B-VII.0 neutron cross section libraries. These libraries contain data for 417 nuclides and 19 thermal-scattering moderators.

Reference [11] contains a more detailed description of the methods used in Insilico as part as the VERA Core Simulator.

3. CODE COUPLING

3.1 Introduction

This paper demonstrates the coupling two physics codes together to calculate the temperature, fission rate, and neutron flux distribution within a PWR core. All neutronics aspects of the problem (cross-sections, neutron transport, and power release) are solved using Insilico and all thermal-hydraulic aspects (including fuel rod conduction) are solved using CTF. The coupling of these codes to create a single-executable multiphysics coupled-code application is done using the VERA infrastructure tools LIME [12][13] and DTK [14].

3.2 Building a Single Executable

To couple the physics codes CTF and Insilico together, both programs are combined and compiled in a single executable using the subroutine interface to CTF and Insilico along with a top-level LIME problem manager. The LIME problem manager serves as the “main” program, controls the iteration strategy, calls the CTF and Insilico subroutines as needed, and transfers data between the codes using LIME model evaluators and DTK (See Figure 3-1 below).

Compiling different physics codes together can be a complicated (and often overlooked) task, especially when the packages are large and rely on additional third-party libraries (TPL’s). To overcome these complications, the TriBITS build system is used.

TriBITS stands for the “Tribal Build, Integrate, and Test System” and was originally developed for Trilinos, but was later extended for VERA, SCALE and other projects. TriBITS is based on the well-known Kitware open-source toolset CMake, CTest, and CDash. TriBITS manages all of the different code packages and TPL’s and provides an integrated build and testing platform for them.

TriBITS is an open-source project and is available for download from the internet [15].

3.3 LIME

The Lightweight Integrating Multiphysics Environment for coupling codes (LIME) is used to integrate the different physics codes into a single application [12][13]. LIME is designed to integrate separate computer codes, which may be written in different languages, into a single application to solve multiphysics problems. LIME provides high-level routines to create a “Problem Manager” to control the overall-iterations and perform communication through “Model Evaluators” for each of the separate physics codes.

A description of how LIME is used to couple CTF and Insilico is provided in Section 3.5.

LIME is an open-source project and is available for download from the internet [16].

3.4 Data Transfer Kit (DTK)

The Data Transfer Kit (DTK) library is used to transfer data between the two physics codes. DTK is based on the Rendezvous algorithm [14] and facilitates the transfer of data between multiple codes with different meshes partitioned on different parallel processors. From the DTK website:

> *“The Data Transfer Kit (DTK) is a software component designed to provide parallel services for mesh and geometry searching and data transfer for arbitrary physics components. In many physics applications, the concept of mesh and geometry is used to subdivide the physical domain into a discrete representation to facilitate the solution of the model problems that describe it. Additionally, the concept of the field is used to apply degrees of freedom to the mesh or geometry as a means of function discretization. With the increased development efforts in multiphysics simulation, adaptive mesh simulations, and other multiple mesh/geometry problems, generating parallel topology maps for transferring fields and other data between meshes is a common operation. DTK is being developed to provide a suite of concrete algorithm implementations for these services.”*

DTK is an open-source project and is available for download from the internet [17].

3.5 Coupling Strategy

A challenging aspect of coupling neutronics and thermal-hydraulics is that the different physics associated with these two codes are strongly coupled and nonlinear. By strongly coupled we mean that the quantities calculated in each physics code and passed to the other have a significant impact on the solution of the other physics code. By nonlinear we mean that a change in values calculated in one code do NOT result in a “linearly-proportional” change to values in the other.

Figure 3-1 illustrates key aspects of the single-executable coupled-code (Insilico-CTF) simulation capability created within VERA to solve this problem.

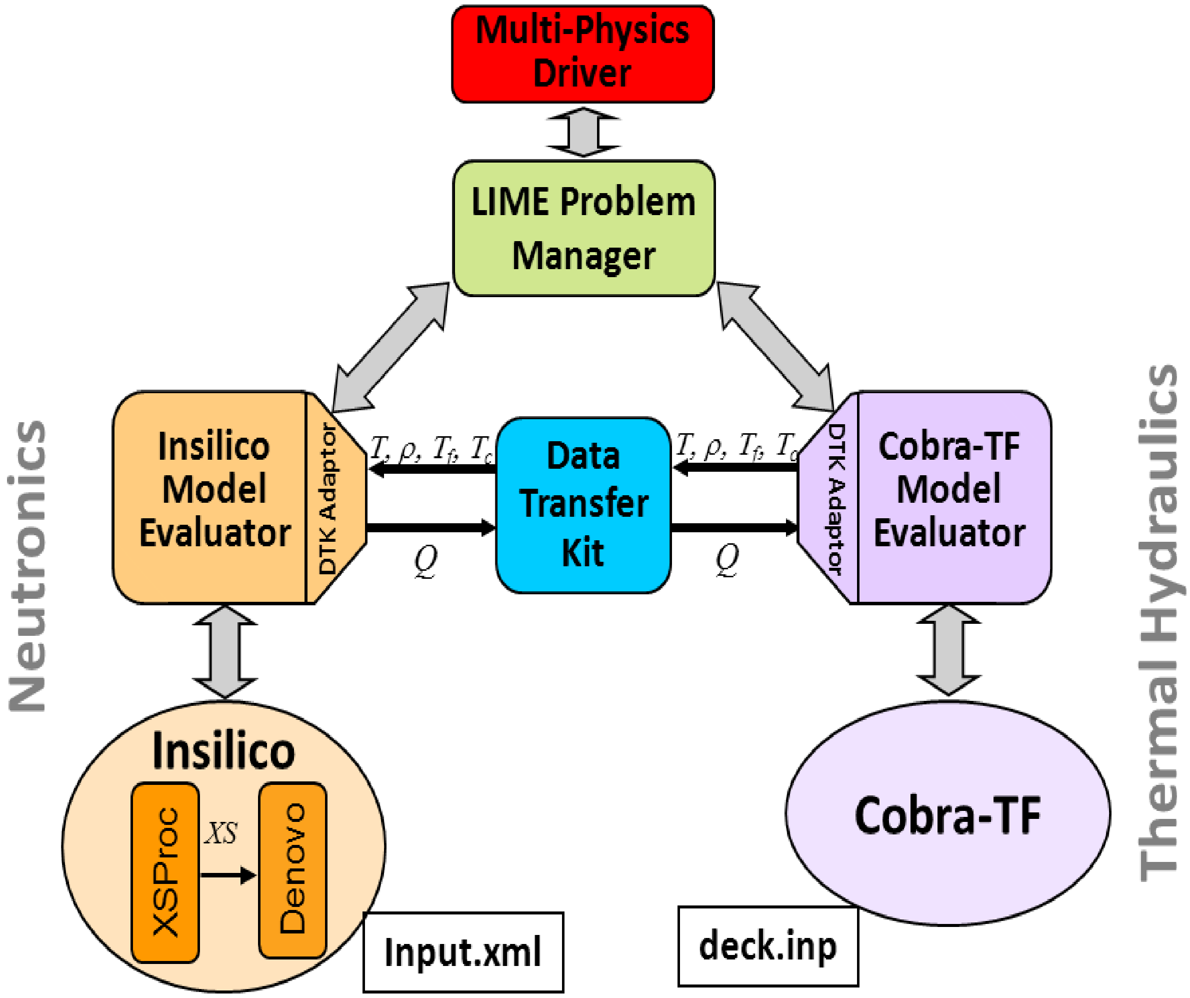

Figure 3-1 Key components of a coupled Insilico-CTF application created to solve the example problem.

To solve the neutronics part of the overall problem, Insilico must be provided with values for the following quantities associated with each rod at each axial level:

1. average fuel temperature, T_f
2. average clad temperature, T_c
3. average coolant temperature surrounding the rod, T_w
4. average coolant density surrounding the rod, ρ_w

These quantities are transferred to Insilico at designated times during the overall solution procedure. Of note is that Insilico is itself solving a multiphysics neutronics problem that involves calculating cross sections, doing neutron transport, and computing energy release.

To solve the thermal hydraulics part of the problem, CTF needs the energy release rate Q in each fuel rod at each axial level. These values are computed by Insilico and transferred to CTF. Note that CTF also solves several coupled-physics equation sets internally, i.e. conservation of mass, momentum and energy in the fluid together with heat transfer to fuel rods where energy is being released and conducted within the rods.

The transfer of data between Insilico and CTF is enabled and directed by several additional software components represented in Figure 3-1 (e.g. Insilico and CTF Model Evaluators and DTK adaptors). These small components leverage LIME and DTK and provide the additional functionality needed to create the overall coupled-code simulation capability. In particular, they address the details of how and where the transfer data are stored in each code, and how to correctly transfer that data in the form required by both the “source” and the “target” during each transfer operation.

As described in references [12] and [13], LIME supports several different types of nonlinear solution strategies (i.e. Newton, Jacobian-free Newton-Krylov (JFNK), fixed point) depending on the capabilities available from the physics codes being coupled. In this case, we solve the overall coupled nonlinear system using a simple “Seidel” mode fixed point algorithm. This is an iterative method where each physics code is sequentially solved independently within a global iteration loop, and updated transfer data are passed between physics codes immediately after each physics code solution. In addition, the change in transferred values between iterations can be “relaxed” so as to improve the convergence of the approach.

The simplified execution diagram in Figure 3-2 illustrates the “Seidel” mode fixed point algorithm executed by the LIME problem manager for our example problem.

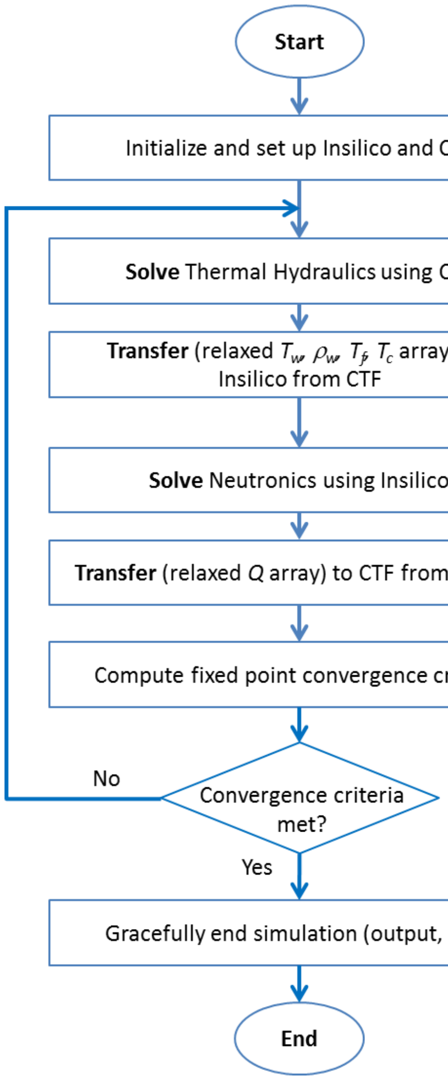

Figure 3-2 Simplified flow chart illustrating the coupled code "Seidel" fixed point algorithm

4. PROBLEM DESCRIPTION

Results are presented for both single-assembly and full-core calculations. The complete geometries are described by the CASL Progression Benchmark Problems Specification [2] and are based on the dimensions and state conditions of Watts Bar Unit 1 Cycle 1.

All dimensions are non-proprietary and are derived from the publically available Watts Bar Unit 1 FSAR [18].

4.1 Single-Assembly Description

The first example problem is a PWR single assembly corresponding to CASL Progression Benchmark Problem 6. Results are shown for different boron concentrations (0, 600, 1300, 3099 ppm) and power levels (70, 100, and 130% power).

The assembly is a standard 17x17 Westinghouse fuel design with uniform fuel enrichment. There are no axial blankets or enrichment zones. The assembly has 264 fuel rods, 24 guide tubes, and a single instrument tube in the center. There are no control rods or removable burnable absorber assemblies in this problem.

The primary geometry specifications of the fuel rod and guide tube materials are given in Table 4-1. The geometry specification for the assembly is given in Figure 4-1 and Table 4-2. The thermal-hydraulic specifications for this problem are shown in Table 4-3. For a complete description of the geometry, including spacer grid and nozzle specifications, refer to the benchmark specifications in reference [2].

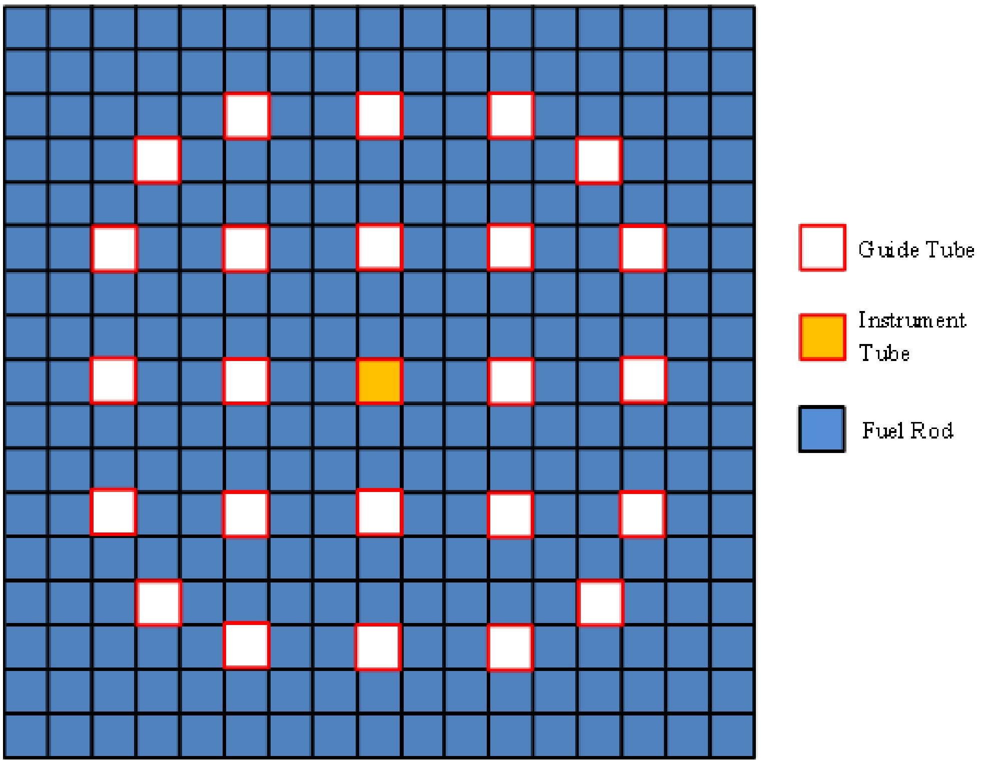

Figure 4-1 Assembly Layout Showing Guide Tubes (GT) and Instrument Tube (IT) placement.

Table 4-1 Fuel Rod and Guide Tube Descriptions

Parameter	Value	Units
Fuel Pellet Radius	0.4096	cm
Fuel Rod Clad Inner Radius	0.418	cm
Fuel Rod Clad Outer Radius	0.475	cm
Guide Tube Inner Radius	0.561	cm
Guide Tube Outer Radius	0.602	cm
Instrument Tube Inner Radius	0.559	cm
Instrument Tube Outer Radius	0.605	cm
Outside Rod Height	385.10	cm
Fuel Stack Height (active fuel)	365.76	cm
Plenum Height	16.00	cm
End Plug Heights (x2)	1.67	cm
Pellet Material	UO_2	
Clad / Caps / Guide Tube Material	Zircaloy-4	

Table 4-2 Assembly Description

Parameter	Value	Units
Rod Pitch	1.26	cm
Assembly Pitch	21.5	cm
Inter-Assembly Half Gaps	0.04	cm
Geometry	17x17	
Number of Fuel Rods	264	
Number of Guide Tubes (GT)	24	
Number of Instrument Tubes (IT)	1	

Table 4-3 Nominal Thermal-Hydraulic Conditions for a Single-Assembly

Parameter	Value	Units
Inlet Temperature	559	degrees F
System Pressure	2250	psia
Rated Flow (100% flow)	0.6824	Mlb/hr
Rated Power (100% power)	17.67	MWt

4.2 Full-Core Description

The second example problem is a full-core PWR corresponding to Progression Benchmark Problem 7. This problem is based on the Watts Bar Unit 1 initial core.

The assembly geometry descriptions for the Watts Bar core are the same as the single-assembly descriptions given in the previous section. The full-core contains 3 enrichment zones (2.1, 2.6, and 3.1% U-235) and several configurations of Pyrex burnable absorber rods. The enrichment zones and Pyrex configurations are shown in Figure 4-3. Additional Core Parameters are shown in Table 4.4. A detailed description of this reactor core is given in [11].

	H	G	F	E	D	C	B	A
8	2.1	2.6 20	2.1	2.6 20	2.1	2.6 20	2.1	3.1 12
9	2.6 20	2.1	2.6 24	2.1	2.6 20	2.1	3.1 24	3.1
10	2.1	2.6 24	2.1	2.6 20	2.1	2.6 16	2.1	3.1 8
11	2.6 20	2.1	2.6 20	2.1	2.6 20	2.1	3.1 16	3.1
12	2.1	2.6 20	2.1	2.6 20	2.6	2.6 24	3.1	
13	2.6 20	2.1	2.6 16	2.1	2.6 24	3.1 12	3.1	
14	2.1	3.1 24	2.1	3.1 16	3.1	3.1		
15	3.1 12	3.1	3.1 8	3.1				

Enrichment
Number of Pyrex Rods

Figure 4-3 Core Layout for Watts Bar Unit 1 Cycle 1

Table 4-4 Full-Core Description

Parameter	Value	Units
Number of Fuel Assemblies	193	
Assembly Pitch	21.5	cm
Inlet Temperature	559	degrees F
System Pressure	2250	psia
Rated Flow (100% flow)	131.68	Mlb/hr
Rated Power (100% power)	3411	MWt

Boron Concentration	1225	ppm
Baffle Gap	0.19	cm
Baffle Thickness (stainless steel)	2.85	cm

5. SINGLE-ASSEMBLY RESULTS

5.1 Modeling Options

All of the single-assembly cases were run on the Titan supercomputer at ORNL using 289 cores (one rod per core). Cross sections are generated with XSProc running pincell calculations (BONAMI and XSDRN) on the fly with the local power, temperatures, and densities. For the single-assembly cases, each pincell calculations is run with 252 energy groups and the macroscopic cross sections are collapsed to 23 energy groups for the 3D transport solution. Insilico uses the SP_3 solver with P_1 scattering, a 2x2 mesh in each fuel rod in the radial direction, and a maximum 1.26 cm mesh in the axial direction. Axial boundaries are positioned at each material and edit interfaces. The neutron flux is calculated from below the lower core plate to above the upper core plate in order to capture the axial leakage effects.

For the T/H solution, CTF uses 49 axial levels over the active fuel region. The axial levels are defined to explicitly include the spacer grid heights, and to use uniform mesh spacing between the spacer grids. The maximum axial mesh is approximately 7 cm. The CTF fuel rod heat conduction model uses 3 radial rings in each fuel rod.

All of the data transfer between Insilico and CTF occurs at each fuel rod on the 49 axial level mesh (the “coupling mesh”)

5.2 Single-Assembly Results

The normalized radial fission rate distribution integrated over the axial direction is shown in Figure 5-1 for the coupled problem. Note that the results are octant symmetric and there is no power in the guide tubes or instrument tubes.

0.946	0.942	0.945	0.954	0.964	0.972	0.972	0.972	0.975	0.972	0.972	0.972	0.964	0.954	0.945	0.942	0.946
0.942	0.940	0.949	0.965	0.985	1.011	0.991	0.990	1.011	0.990	0.991	1.011	0.985	0.965	0.949	0.940	0.942
0.945	0.949	0.974	1.016	1.037		1.026	1.025		1.025	1.026		1.037	1.016	0.974	0.949	0.945
0.954	0.965	1.016		1.052	1.042	1.011	1.008	1.030	1.008	1.011	1.042	1.052		1.016	0.965	0.954
0.964	0.985	1.037	1.052	1.035	1.043	1.014	1.011	1.034	1.011	1.014	1.043	1.035	1.052	1.037	0.985	0.964
0.972	1.011		1.042	1.043		1.037	1.036		1.036	1.037		1.043	1.042		1.011	0.972
0.972	0.991	1.026	1.011	1.014	1.037	1.013	1.012	1.036	1.012	1.013	1.037	1.014	1.011	1.026	0.991	0.972
0.972	0.990	1.025	1.008	1.011	1.036	1.012	1.012	1.036	1.012	1.012	1.036	1.011	1.008	1.025	0.990	0.972
0.975	1.011		1.030	1.034		1.036	1.036		1.036	1.036		1.034	1.030		1.011	0.975
0.972	0.990	1.025	1.008	1.011	1.036	1.012	1.012	1.036	1.012	1.012	1.036	1.011	1.008	1.025	0.990	0.972
0.972	0.991	1.026	1.011	1.014	1.037	1.013	1.012	1.036	1.012	1.013	1.037	1.014	1.011	1.026	0.991	0.972
0.972	1.011		1.042	1.043		1.037	1.036		1.036	1.037		1.043	1.042		1.011	0.972
0.964	0.985	1.037	1.052	1.035	1.043	1.014	1.011	1.034	1.011	1.014	1.043	1.035	1.052	1.037	0.985	0.964
0.954	0.965	1.016		1.052	1.042	1.011	1.008	1.030	1.008	1.011	1.042	1.052		1.016	0.965	0.954
0.945	0.949	0.974	1.016	1.037		1.026	1.025		1.025	1.026		1.037	1.016	0.974	0.949	0.945
0.942	0.940	0.949	0.965	0.985	1.011	0.991	0.990	1.011	0.990	0.991	1.011	0.985	0.965	0.949	0.940	0.942
0.946	0.942	0.945	0.954	0.964	0.972	0.972	0.972	0.975	0.972	0.972	0.972	0.964	0.954	0.945	0.942	0.946

Figure 5-1 Normalized Radial Fission Rate Distribution at 1300 ppm and 100% power

A map of the coolant density in the top axial elevation of each channel is shown in Figure 5-2. Note that the exit density is lower in the center of the assembly, corresponding to the higher fuel rod powers shown in Figure 5-1.

0.659	0.658	0.658	0.657	0.656	0.656	0.655	0.655	0.655	0.655	0.655	0.655	0.656	0.656	0.657	0.658	0.658	0.659
0.658	0.658	0.657	0.656	0.656	0.655	0.655	0.655	0.655	0.655	0.655	0.655	0.655	0.656	0.656	0.657	0.658	0.658
0.658	0.657	0.656	0.656	0.655	0.655	0.654	0.654	0.654	0.654	0.654	0.654	0.655	0.655	0.656	0.656	0.657	0.658
0.657	0.656	0.656	0.655	0.655	0.654	0.653	0.653	0.653	0.653	0.653	0.653	0.654	0.655	0.655	0.656	0.656	0.657
0.656	0.656	0.655	0.655	0.654	0.653	0.653	0.652	0.652	0.652	0.652	0.653	0.653	0.654	0.655	0.655	0.656	0.656
0.656	0.655	0.655	0.654	0.653	0.653	0.652	0.652	0.652	0.652	0.652	0.652	0.653	0.653	0.654	0.655	0.655	0.656
0.655	0.655	0.654	0.653	0.653	0.652	0.652	0.652	0.652	0.652	0.652	0.652	0.652	0.653	0.653	0.654	0.655	0.655
0.655	0.655	0.654	0.653	0.652	0.652	0.652	0.651	0.651	0.651	0.651	0.652	0.652	0.652	0.653	0.654	0.655	0.655
0.655	0.655	0.654	0.653	0.652	0.652	0.652	0.651	0.652	0.652	0.651	0.652	0.652	0.652	0.653	0.654	0.655	0.655
0.655	0.655	0.654	0.653	0.652	0.652	0.652	0.651	0.652	0.652	0.651	0.652	0.652	0.652	0.653	0.654	0.655	0.655
0.655	0.655	0.654	0.653	0.652	0.652	0.652	0.651	0.651	0.651	0.651	0.652	0.652	0.652	0.653	0.654	0.655	0.655
0.655	0.655	0.654	0.653	0.653	0.652	0.652	0.652	0.652	0.652	0.652	0.652	0.652	0.653	0.653	0.654	0.655	0.655
0.656	0.655	0.655	0.654	0.653	0.653	0.652	0.652	0.652	0.652	0.652	0.652	0.653	0.653	0.654	0.655	0.655	0.656
0.656	0.656	0.655	0.655	0.654	0.653	0.653	0.652	0.652	0.652	0.652	0.653	0.653	0.654	0.655	0.655	0.656	0.656
0.657	0.656	0.656	0.655	0.655	0.654	0.653	0.653	0.653	0.653	0.653	0.653	0.654	0.655	0.655	0.656	0.656	0.657
0.658	0.657	0.656	0.656	0.655	0.655	0.654	0.654	0.654	0.654	0.654	0.654	0.655	0.655	0.656	0.656	0.657	0.658
0.658	0.658	0.657	0.656	0.656	0.655	0.655	0.655	0.655	0.655	0.655	0.655	0.655	0.656	0.656	0.657	0.658	0.658
0.659	0.658	0.658	0.657	0.656	0.656	0.655	0.655	0.655	0.655	0.655	0.655	0.656	0.656	0.657	0.658	0.658	0.659

Figure 5-2 Exit Coolant Density (g/cc) at 1300 ppm and 100% power

Average axial distributions for this problem are shown in Figures 5-3. Note the small "dips" in the axial fission rate and fuel temperature profiles. These dips are due to the presence of spacer grids. The spacer grids displace moderator in the coolant channels and decrease the neutron moderation around the grids. The decreased moderation causes a local depression in the flux and power.

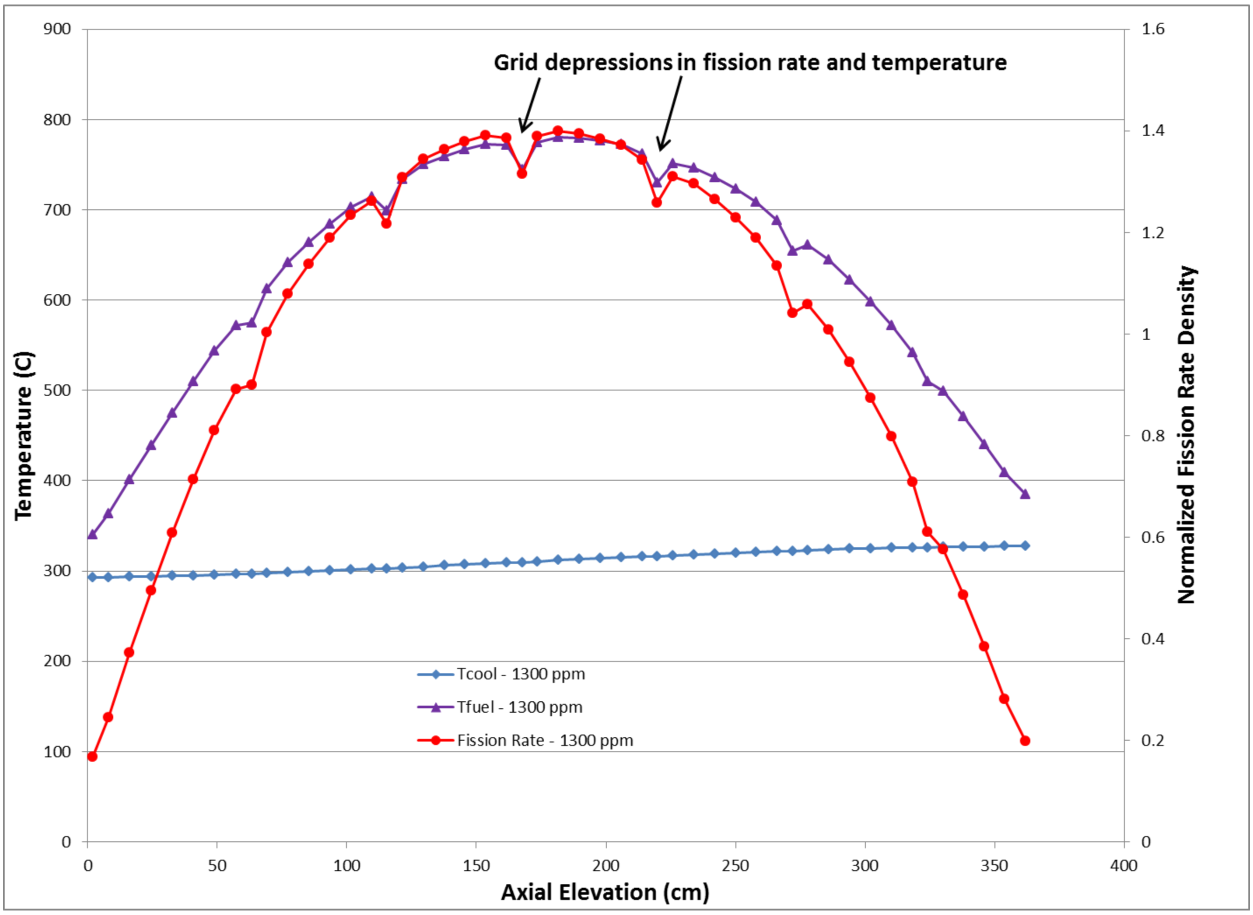

Figure 5-3 Axial Distributions at 1300 ppm and 100% power (with fuel temperature shown)

5.3 Boron Perturbations

To see the effects of different boron concentrations on the results, the single-assembly case was run at four different boron concentrations – 0, 600, 1300, and 3099 ppm boron. The eigenvalues and wall-clock times for these cases are listed in Table 5-2.

Table 5-2 Iteration Summary for Boron Cases

Boron Concentration	Eigenvalue	Wall Time (HH:MM:SS)	Coupled Iterations
0 ppm	1.32797	2:13:39	9
600 ppm	1.24634	2:18:10	10
1300 ppm	1.16421	2:08:36	9
3099 ppm	1.00000	2:58:30	13

The fission rate and fuel temperature profiles for three different boron concentrations are shown in Figure 5-4.

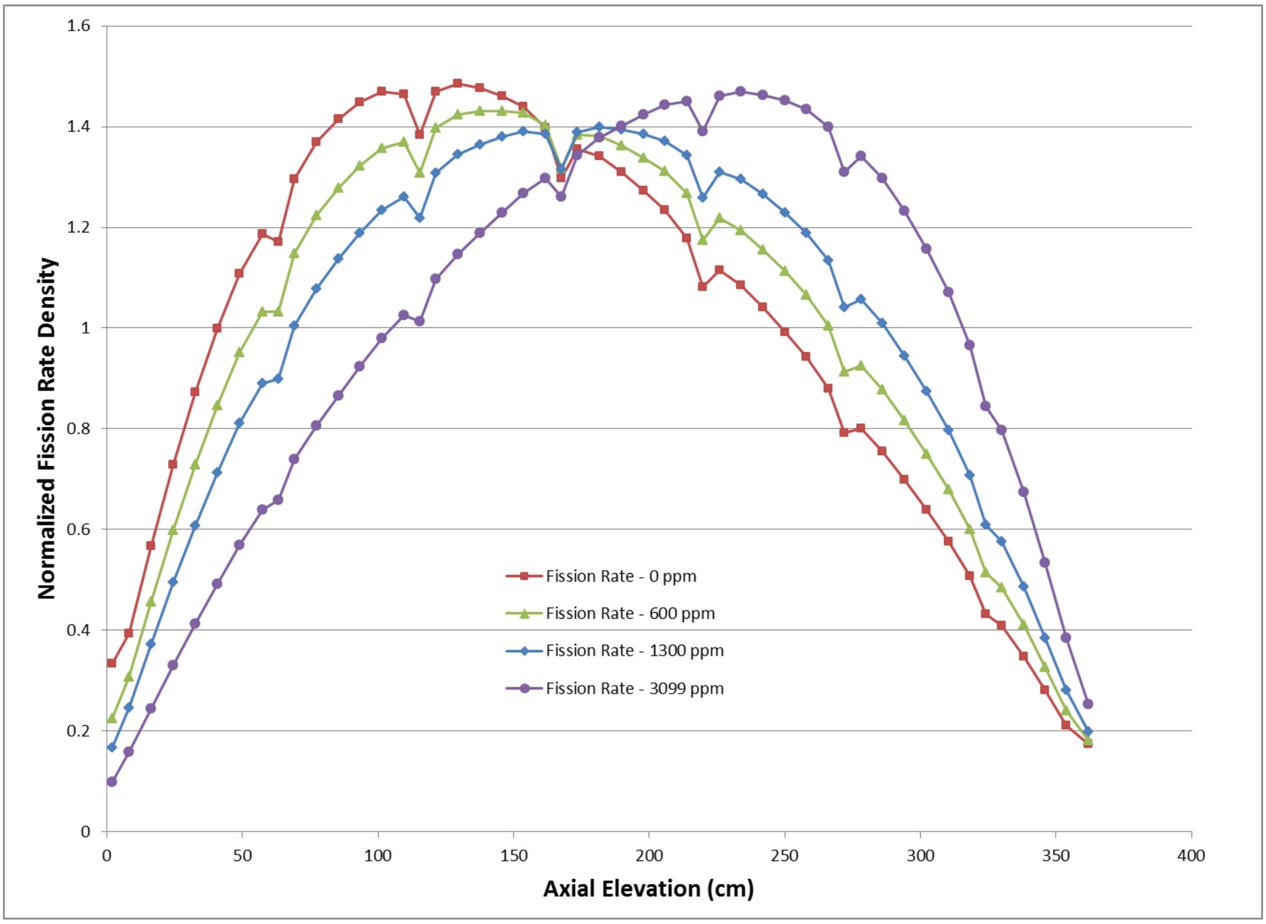

Figure 5-4 Axial Plot of Fission Rates at Different Boron Concentrations

5.4 Power Perturbations

To see the effects of different power levels on the results, the nominal single-assembly case was run at three different power levels – 70, 100, and 130% power. The eigenvalues and wall-clock times for these cases are shown in Table 5-3.

Table 5-3 Iteration Summary for Power Cases

Power Level	Eigenvalue	Wall Time (HH:MM:SS)	Coupled Iterations
70%	1.25235	2:30:10	11
100%	1.24634	2:18:10	10
130%	1.23993	2:34:07	11

The fission rate profiles for the four power cases are shown in Figure 5-7. At higher power levels, the fission rate shape is shifted lower in the core from the normal cosine-shaped distribution you would see with no T/H feedback.

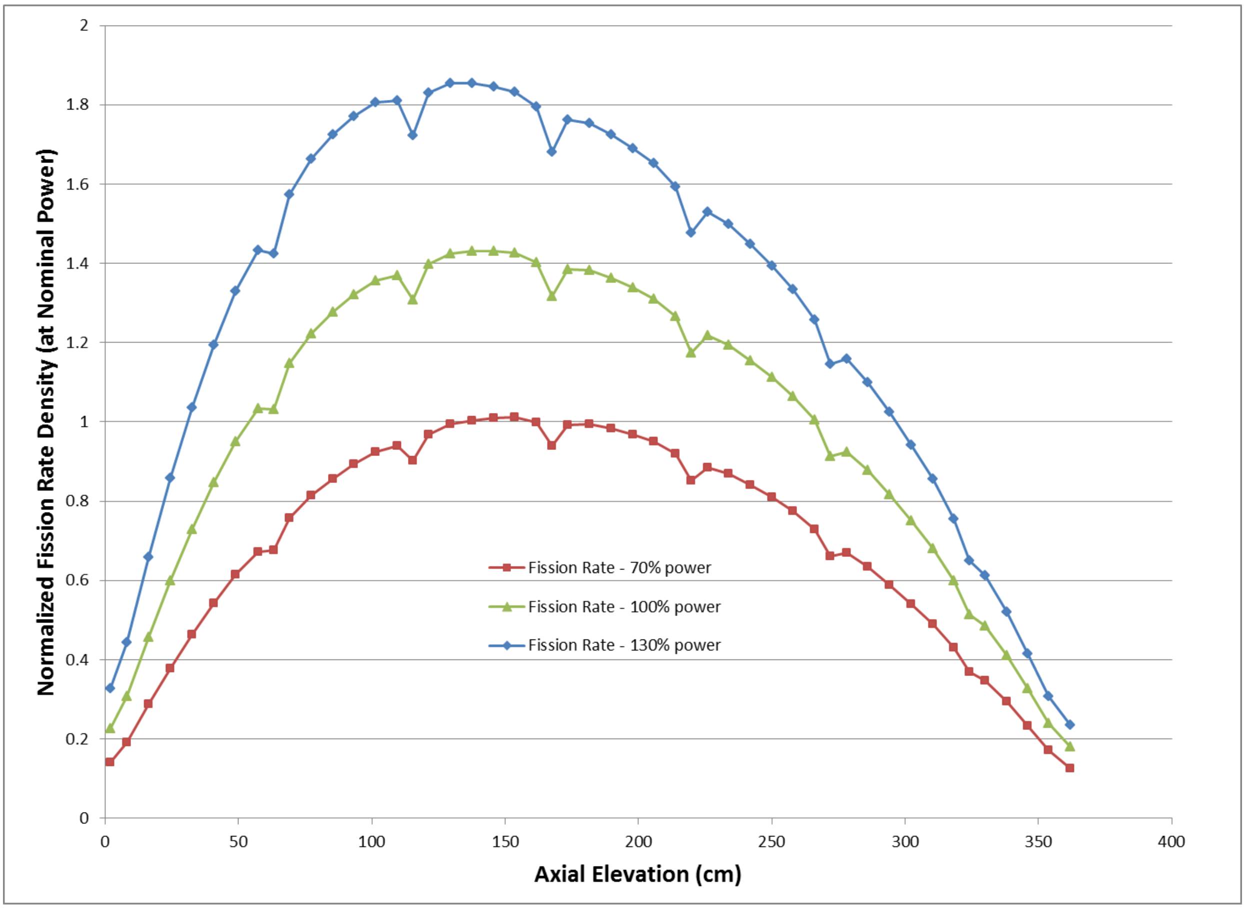

Figure 5-7 Axial Plot of Fission Rates at Different Power Levels

6. FULL-CORE RESULTS

This section contains results for a full-core model run with a coupled Insilico-CTF solver using quarter-core symmetry.

6.1 Full-Core Modeling Options

The full-core results were run on Titan using 18,769 cores (137x137 – approximately one rod per core).

The neutronics solution was generated with Insilico using cross sections from XSProc and the SP_N 3D transport solver. XSProc generates cross sections for each unique region by running a 56-group pincell calculation (BONAMI and XSDRN) for each region and spatially averaging the cross sections over the fuel rod and collapsing to 11 energy groups for the 3D transport solve. The 3D SP_N solver uses a SP_3 solution with P_1 scattering, a 2x2 mesh in each fuel rod, and a maximum axial mesh of 7.62 cm. Axial boundaries are positioned at each material and coupling interface. The neutron flux is calculated from below the lower core plate to above the upper core plate in order to capture the axial leakage effects.

The T/H solution is generated with CTF using 49 axial levels in the active fuel region. The axial levels are defined to explicitly include the spacer grid heights, and to use uniform mesh spacing between the spacer grids. The maximum axial mesh in CTF is approximately 7 cm. The CTF fuel rod heat conduction model uses 3 radial rings in each fuel rod.

Data transfer between Insilico and CTF occurs at each fuel rod on the 49 axial level mesh (the "coupling mesh").

6.2 Full-Core Results

The iteration summary for two full-core calculations is shown in Table 6-1. The 1285 ppm case was run first and the run-time shown is the sum of two smaller runs. The first of the smaller runs ran 7 iterations before exceeding the maximum run-time limits on Titan. This case was re-started and took an additional 3 iterations to converge.

To speed up the calculation of the 800 ppm case, the initial power distribution was initialized using the final power distribution from the 1285 ppm case. This reduced the number of iterations needed to converge and allowed the case to avoid the run-time limits on Titan.

Table 6-1 Iteration Summary for Full-Core Cases

Boron Concentration	Eigenvalue	Wall Time (HH:MM)	Coupled Iterations
800 ppm	1.03123	10:14*	9
1285 ppm	0.98310	14.39	10

* This case was started using an initial power distribution from the 1285 ppm case

The 2D assembly power results (axially integrated and assembly averaged) are shown in Figure 6-1. The maximum relative assembly power is 1.2758 and the minimum relative assembly power is 0.6337, which occurs on the core boundary.

The minimum and maximum pin power results are shown in Table 6-2. A plot of the maximum, minimum, and average axial rod powers is shown in Figure 6-2.

	H	G	F	E	D	C	B	A
8	1.0619	0.9815	1.0605	1.0222	1.1330	1.0491	1.0550	0.7740
9	0.9815	1.0500	0.9428	1.1053	1.0612	1.1452	1.0334	0.8806
10	1.0605	0.9428	1.0856	1.0489	1.1641	1.1257	1.0682	0.7859
11	1.0222	1.1053	1.0489	1.1592	1.0830	1.1298	1.0218	0.6516
12	1.1330	1.0612	1.1641	1.0830	1.2758	0.8979	0.9334	
13	1.0491	1.1452	1.1257	1.1298	0.8979	0.9134	0.6337	
14	1.0550	1.0334	1.0682	1.0218	0.9334	0.6337		
15	0.7740	0.8806	0.7859	0.6516				

Figure 6-1 2D Assembly Power Results for 1285 ppm case

Table 6-2 Pin Power Results for 1285 ppm

	Power	Pin Location	Level	Assembly
2D min rod	0.1544	(4,5)	--	C-14/B-13
2D max rod	1.3981	(17,17)	--	D-12
3D min	0.0246	(4,5)	1	C-14/B-13
3D max	1.9756	(17,17)	20	D-12

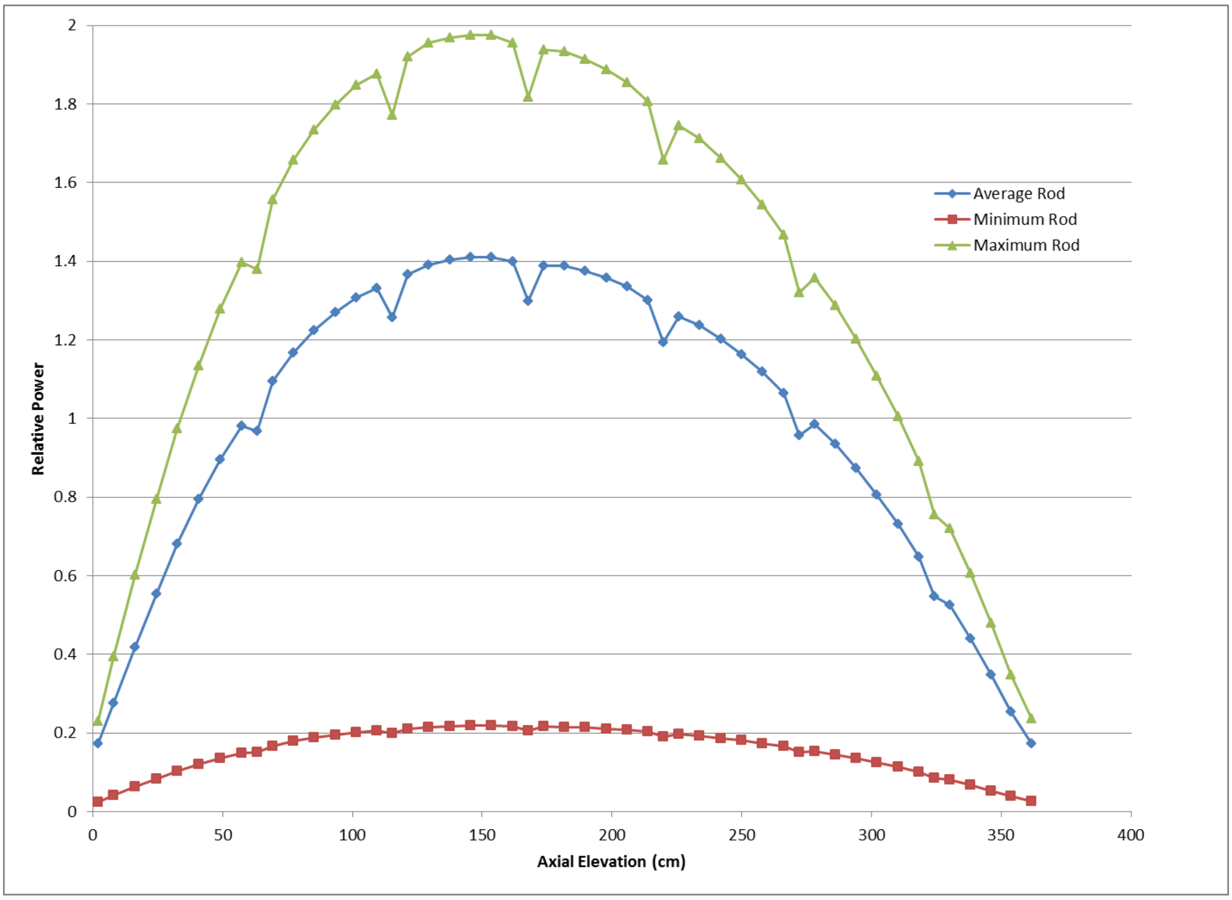

Figure 6-2 Axial Plots of Maximum, Minimum, and Average Rod Powers

Figure 6-3 shows the 3D thermal flux distribution for this problem. The top of the core has been removed from the plot to show the flux distribution in the fuel. The thermal flux is defined as the flux below 0.625 eV. Since most fissions occur at thermal energies, the thermal flux is closely related to the power. From this figure, you can observe the assemblies with Pyrex absorber rods have a lower thermal flux (and power). This figure also shows that the thermal flux is also suppressed around the axial grid spacers.

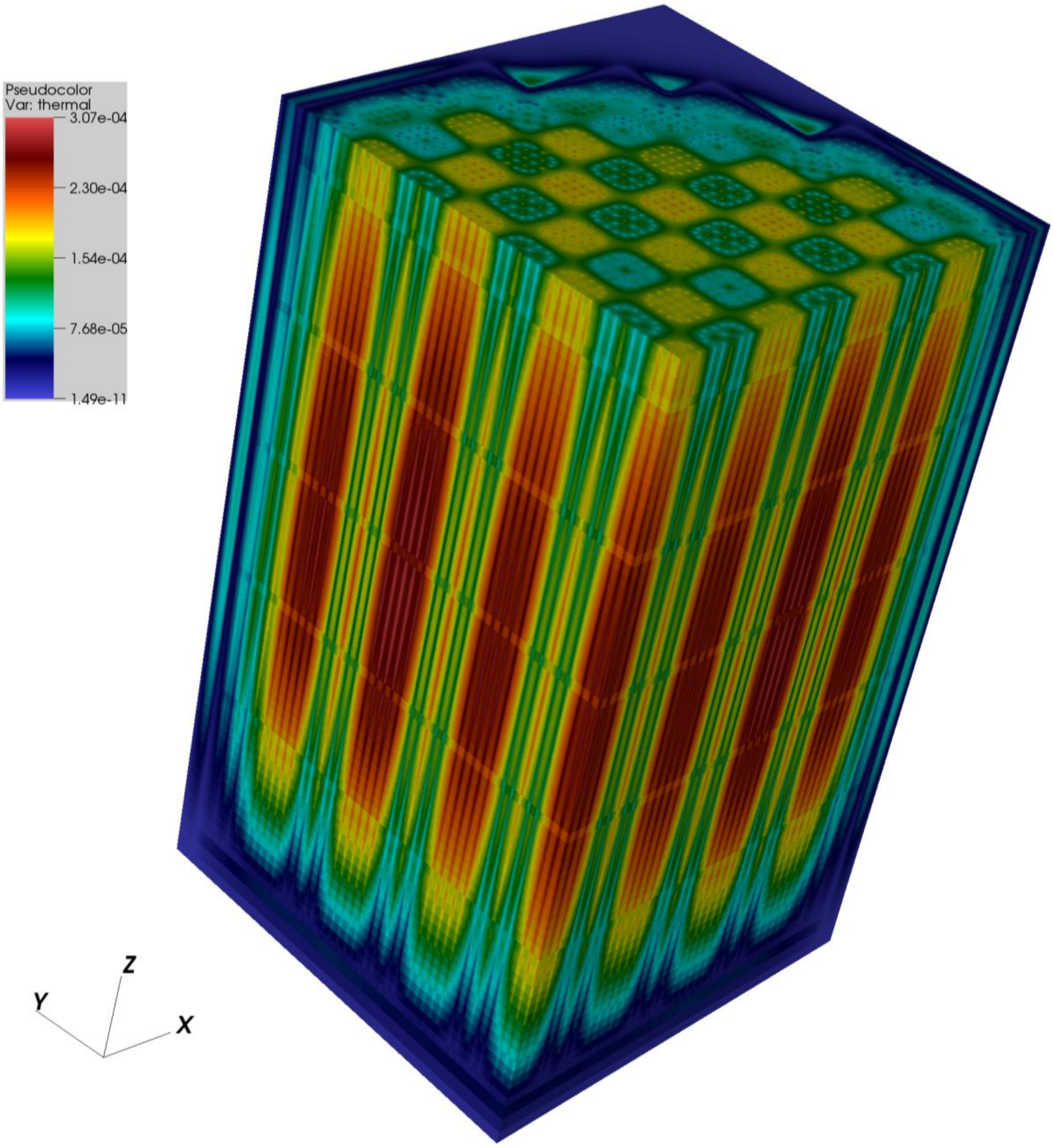

Figure 6-3 3D Thermal Flux Distribution with a cutout at the top of the core

Figure 6-4 shows a 2D slice of the thermal flux near the core midplane. In this figure you can observe where the Pyrex rods are located and you can also see the thermal flux “wings” in the radial reflector region.

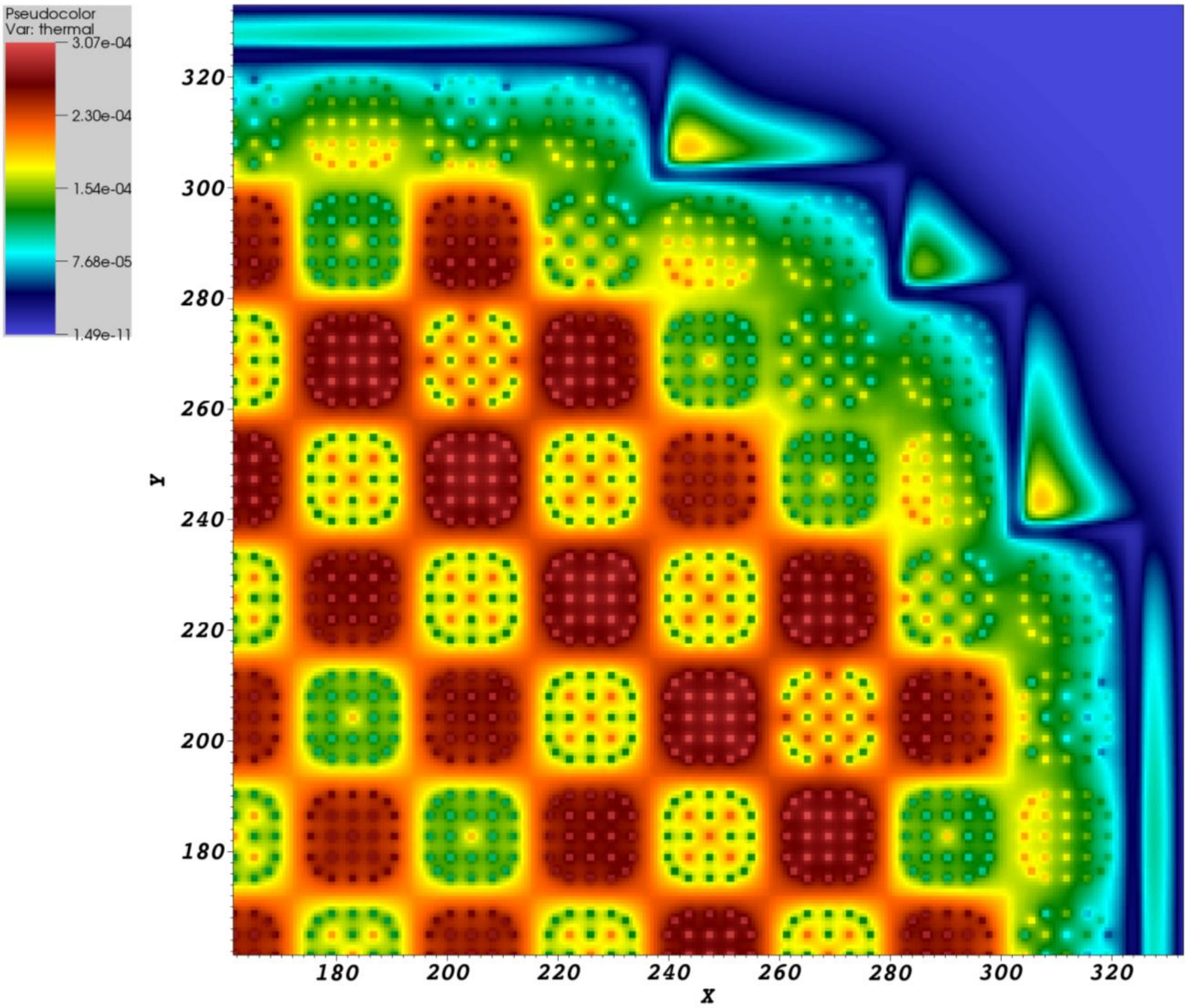

Figure 6-4 2D Slice of Thermal Flux Distribution near the Core Midplane

Figure 6-5 shows a 3D figure of the coolant enthalpy in the active fuel region. This figure shows that the enthalpy rise is not uniform and is closely related to the assembly powers.

Figure 6-6 shows a 2D figure of the coolant enthalpy at the core exit. Note the large enthalpy gradients at the core periphery.

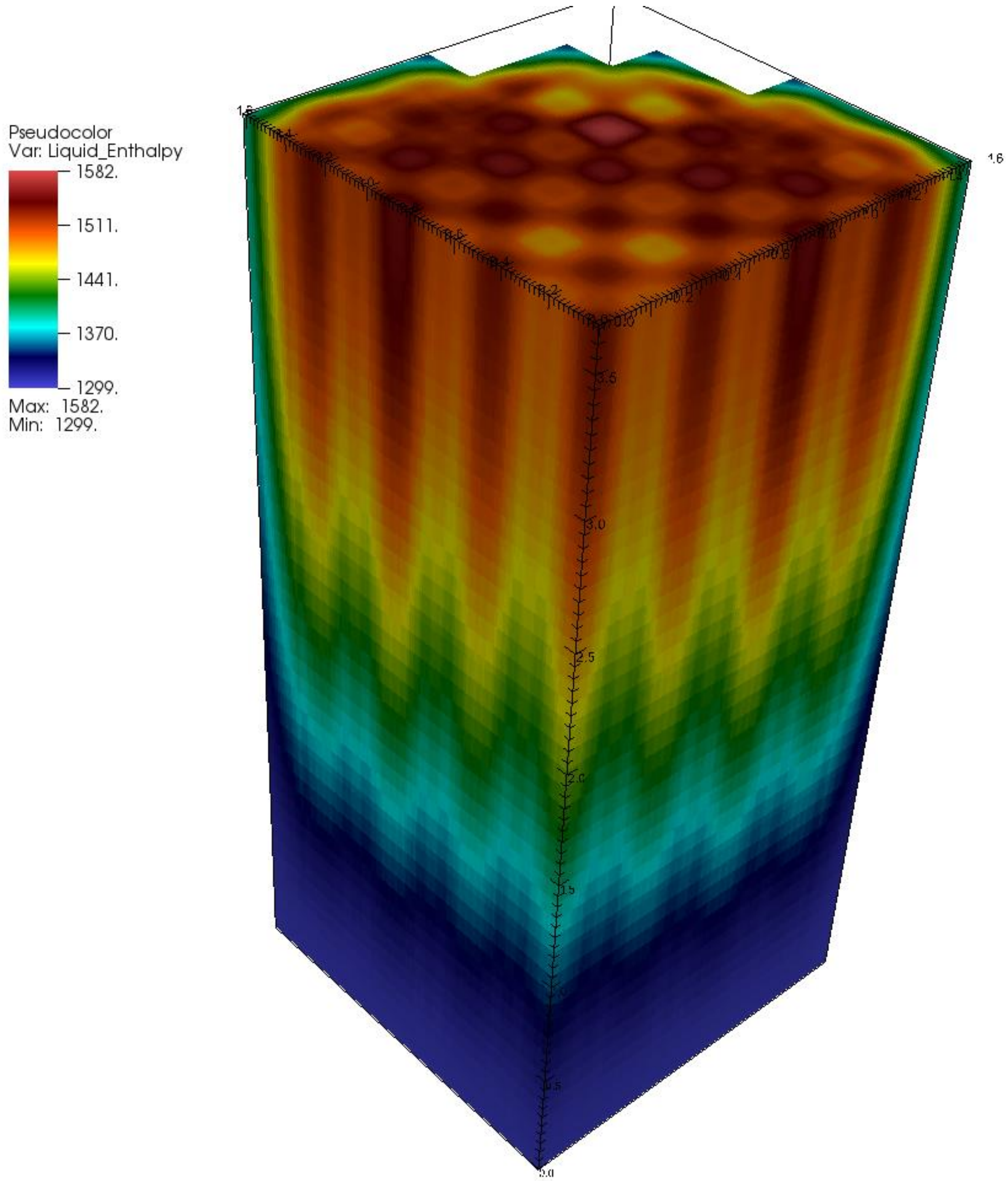

Figure 6-5 3D Coolant Enthalpy Distribution in the active fuel region

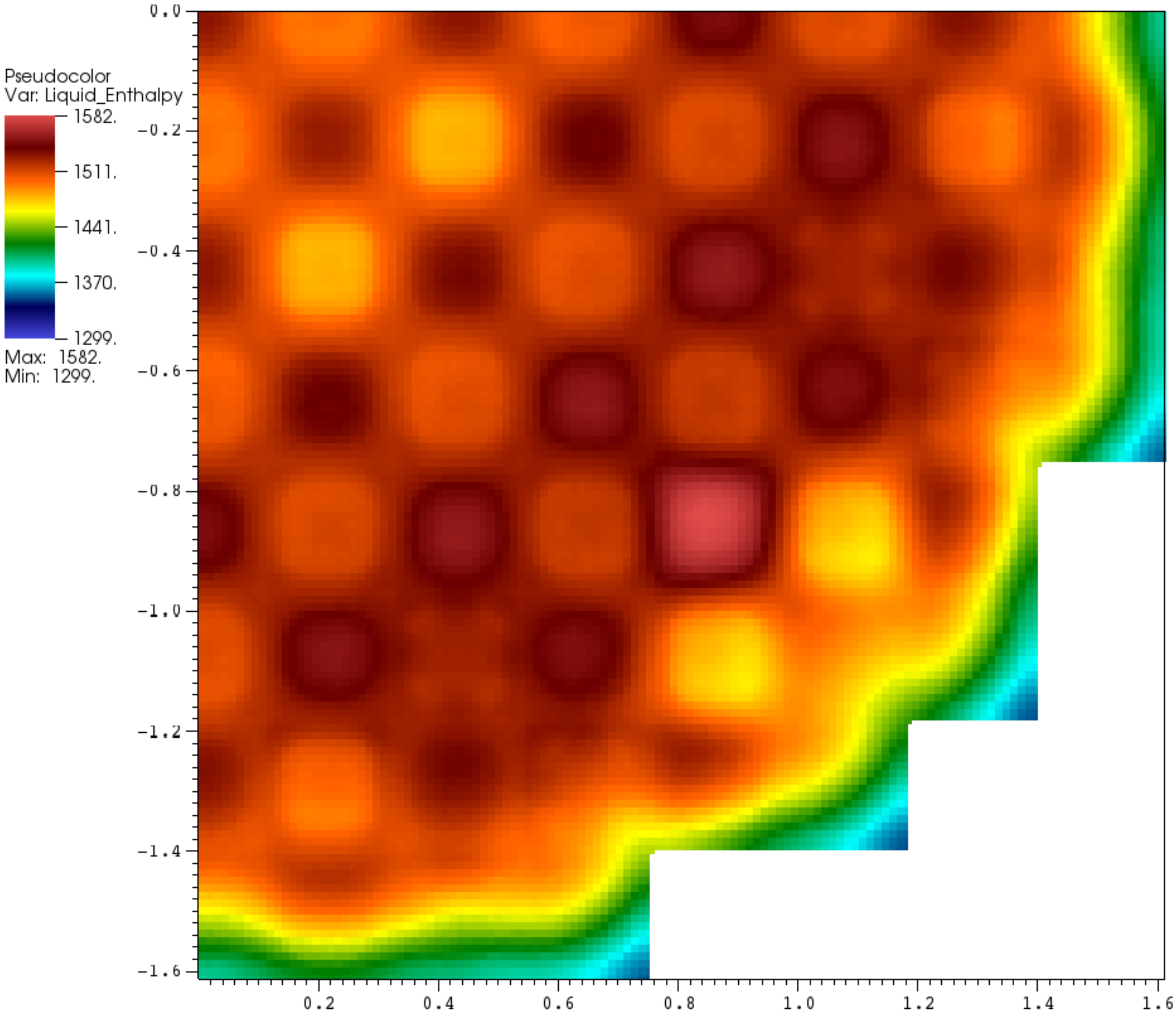

Figure 6-6 Coolant Enthalpy Distribution at the Core Exit

7. CONCLUSION

This paper demonstrates the successful multiphysics coupling of the Insilico neutronics code to the CTF thermal-hydraulics code for a full-core operating reactor. Multiphysics results are shown for several single-assembly cases (CASL Progression Benchmark 6) and for a full-core operating reactor based on Watts Bar Unit 1 Cycle 1 (CASL Progression Benchmark 7).

CASL now has the capability to model full-core reactors at HFP conditions with:

- 3-D pin-by-pin neutron transport (pin homogenized),
- Multigroup cross sections generated for each unique pincell region with local densities and temperatures,
- 3D subchannel T/H calculations for each rod subchannel in the core, and
- 3D pin-by-pin fuel temperature distributions.

This capability is a significant advance over current industry nodal methods which typically have neutronics, cross section, and T/H resolution of a quarter-assembly (which is typically 8.5 pins by 8.5 pins).

Additional development is in progress to complete CASL Progression Benchmarks 8-10 to extend the VERA-CS capability to pin-resolved neutron transport, depletion, and core shuffling.

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